

Development of a Consistent Multi-Sensor Global Ocean Color Time Series

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Abstract

The SIMBIOS (Sensor Intercomparison and Merger for Biological and Interdisciplinary Oceanic Studies) Program was developed to provide a long-term ocean color data set that encompasses the measurements from several satellite instruments. As such, the program is designed to serve as a bridge between previous, current, and future ocean color missions. The previous missions include the Ocean Color and Temperature Scanner (OCTS) and the Polarization and Directionality of the Earth's Reflectances (POLDER) instrument on ADEOS-I. The current missions include the Modular Optoelectronic Scanner (MOS) on IRIS-P3, the Sea-viewing Wide Field-of-view Sensor (SeaWiFS) onboard OrbView2, the Moderate Resolution Imaging Spectroradiometer (MODIS) and the Multi-angle Imaging SpectroRadiometer (MISR) on Terra. The future missions include MODIS on Aqua, the Medium Resolution Imaging Spectrometer (MERIS) onboard Envisat, and the Global Imager (GLI) and POLDER-II on ADEOS-II. To accomplish this, SIMBIOS has adopted the MOBY (Marine Optical Buoy) ocean platform and the SeaWiFS atmospheric correction algorithm as common references for measurements from the different instruments. This approach by SIMBIOS does not preclude other ocean color reference sites or atmospheric correction procedures. Indeed, it is anticipated that future developments, particularly improvements to atmospheric correction algorithms, will supercede the current references. The MOBY buoy, however, provides an exceptional set of water-leaving radiances for the intercomparison and merger of measurements from instruments on different satellite platforms. These measurements are traceable to the National Institute of Standards and Technology (NIST), the metrology laboratory for the United States, providing a long-term repeatability for the data set. To date, measurements by OCTS, POLDER, and SeaWiFS have been compared with MOBY to provide a uniform set of ocean color measurements at a single site. In addition, the SeaWiFS Bio-optical Archive and Storage System (SeaBASS) is used by SIMBIOS to provide a set of *in situ* (field collected) water leaving radiance and chlorophyll-*a* measurements for the validation of satellite ocean color measurements at locations away from the MOBY site. SeaBASS and the Aerosol Robotic Network (AERONET) archive also include an extensive set of *in situ* measured aerosol optical thicknesses and other atmospheric parameters to provide a basis for examining and improving current atmospheric correction algorithms. All of these components can be combined using the SeaWiFS Data Analysis System (SeaDAS), which is in continuing development and is closely linked to the SeaWiFS and SIMBIOS Projects. SeaDAS allows the user to ingest, process, and display ocean color measurements from different satellite sensors. Currently, SeaDAS can work with data from the Coastal Zone Color Scanner (CZCS), OCTS, POLDER, MOS, and SeaWiFS and can be used to display MODIS data. Planning is underway for the enhancement of SeaDAS to display data from POLDER-II, GLI, and MERIS. In addition, SeaDAS has the capacity to modify a number of atmospheric parameters to provide alternate atmospheric corrections for these measurements. This makes SeaDAS an excellent tool for the testing of upgraded and improved atmospheric correction algorithms. Finally, the SIMBIOS Science Team is working on the optimal procedure for combining the OCTS, POLDER, MOS, MODIS, and SeaWiFS measurements into a single, global ocean color data set as a precursor to an expanded data set that includes other current and future satellite instruments. There is a proposed climatology that provides monthly global chlorophyll-*a* and related ocean color fields on a 9 kilometer grid, using a blend of *in situ* and satellite measurements. The use of MOBY as a normalizing reference for this time series should remove problems with the selection of an appropriate reference from the set of satellite instruments.

Keywords: Data set, ocean color, multi-satellite, global, long-term

1. Introduction

For Earth observations from space there is a distinction between monitoring (the routine observation of processes for operational forecasting, early warning, or management) and long-term science (the study of environmental processes that

occur on long time scales). The SIMBIOS Program, which is modeled after the SeaWiFS Project, is designed in part to serve the latter purpose by developing a consistent time series of ocean color from multiple satellite sensors. In addition, the program gathers *in situ* information to support satellite measurements. The ocean color data from these measurements will serve as a framework for scientific studies of ocean ecosystems.

The science issues behind ocean color studies can be summarized as three broad objectives. The first is the characterization of the variability, both spatial and temporal, in the structure of the phytoplanktonic community and its links with higher trophic levels as well as with ocean biochemistry. The second is the prediction of the ocean's biogeochemical response to and its influence on climatic change. And the third is the development of the scientific basis necessary to manage the sustainable resources of the coastal marine ecosystem effectively. In addition to providing measurements of the distribution of phytoplankton, ocean color data can be used to provide estimates of some important ocean processes relevant to air-sea fluxes, particularly primary productivity. An understanding of the patterns in ocean biology will provide a basis for an understanding of biological processes within the ocean.

Biomass turnover rates for plankton ecosystems are one hundred times faster than those for terrestrial ecosystems, leading to a close relationship between upper-ocean ecology and physical forcing. For example, coupled ocean and atmospheric models show that changes in the phytoplanktonic community structure and the resulting elemental interactions can drastically affect the rate of carbon dioxide increase in the atmosphere. Ocean ecosystems also change on decadal time scales in response to climate change. Moreover, the large time and space scales associated with ocean biogeochemistry and circulation can be disrupted on intermediate time scales, such as those of the El Niño/Southern Oscillation. This coupling of large and small time scales leads to the fundamental sampling requirement of global-scale, long-time series (decades) at moderate time and spatial scales (days and kilometers).

Currently, the fundamental geophysical products are diffuse attenuation, phytoplankton chlorophyll-*a*, CDOM, and suspended sediments. New MODIS products include chlorophyll fluorescence, calcite, and primary productivity. However, it is expected that this list will expand as more complete *in situ* measurements and semi-analytical models allow new parameters to be estimated. Currently most products are based on empirical correlations between the ratios of water-leaving radiances at a few wavelengths. A more rigorous approach to the application of ocean color measurements will come from an understanding of the inherent optical properties of each of the optically significant components of seawater.

It is clear that many, if not most, Earth science problems require an interdisciplinary approach for their understanding and prediction. For studies of ocean primary productivity, for example, there are preliminary models of how various physical processes affect light and nutrient availability for phytoplanktonic communities (NASA, 1987). The patterns of primary forcing, as well as the patterns of ocean color, will be necessary to provide the patterns of primary production – and, ultimately, to provide an understanding of the key mechanisms behind the processes.

No single data set will suit all scientific requirements. Studies of river mouths and estuaries will require measurements with spatial sampling requirements that challenge global satellite sensors. And studies of coastal ocean processes will require far more intensive temporal sampling than the open ocean, because of their small characteristic scales. For example, tidal forcing is an important component of the coastal environment, and satellite measurements from sun-synchronous orbits will shift this high-frequency variability into lower frequencies (NRC, 2000a). Ultimately, individual ocean color data sets must be constrained by their applicability to one or a few related Earth science problems.

Finally, the generation system for the data set must be constructed in a manner that scientists not directly involved in its establishment can contribute to the development of new algorithms and new data (NRC, 1995). Accessibility by the fullest possible user community is critical for the maximum use of the data and for meeting the science objectives for the data set. For more than a decade, the SeaWiFS Data Analysis System (SeaDAS) (Baith et al., 2001) has developed user friendly data processing and display software for several ocean color instruments, including CZCS, SeaWiFS, OCTS, POLDER, MODIS, and MOS. This software is freely available for download from the SeaDAS website (<http://seadas.gsfc.nasa.gov>), and it has the flexibility to provide executable programs for those who only need the basic capabilities as well as source code for those who wish adapt the code to insert alternate algorithms. The SeaDAS team, with the assistance of the SeaWiFS and SIMBIOS Projects, is working to develop new ocean color data products and enhanced accessibility to these data for an expanding user community.

The ideas presented in this introduction are not unique to the SIMBIOS Program, nor, for the most part, were they originated by the project. To a large extent, these ideas are direct reflections of issues and recommendations in reports of the National Research Council (NRC, 1995, 1999a, 1999b, 2000a, 2000b), which provide guidelines to NASA for long-term climate data sets.

2. Ocean Color Program Objectives

Individual spaceborne ocean color sensors, including SeaWiFS, routinely measure meso-scale oceanic phenomena, such as the phytoplankton bloom around the Marquesas Islands (Signorini et al. 1999), where the bloom extended from 500 to 1000 km downstream of the islands in the flow of the South Equatorial Current. These sensors can also measure the

variability of chlorophyll-*a* on basin scales (Murtugudde et al. 1999) and can provide measurements of the near surface phytoplankton chlorophyll-*a* concentration globally over the time scale of the El Niño/Southern Oscillation (Behrenfeld et al. 2001). Indeed, models of oceanic primary production have been greatly aided by global-scale satellite observations of phytoplankton biomass (Field et al. 1998) – as have terrestrial models by remote sensing of the land. A long-term, multi-platform ocean color data set must provide the basis for studies such as these, and more, particularly for studies over time scales that extend beyond the operational lifetimes of individual sensors.

The coordination of a long-term ocean color data set by the SIMBIOS Program, with guidance from the International Ocean-Colour Coordinating Group (IOCCG), is a scientific and technological experiment requiring collaboration by the international community. The development of the data set as a research tool must be focused on a set of key unanswered scientific questions – questions about the ocean environment that will be used to formulate the observations and analyses required for their resolution. Without this focus, research on the complex and varied ocean system is likely to be fragmented and inconclusive. However, this focus must be balanced by the knowledge that there will be surprises in future ocean color research. The data set must be sufficiently broad to catch the unexpected, if that is possible (NRC, 1999a). This balance is a principal challenge to the coordination of the data set. In addition, answers to the key scientific questions will require an interdisciplinary approach, since oceanic biological processes are complex. The ocean color data set cannot stand alone. It must be coordinated with other atmospheric and oceanic observations.

2.1. Science Objectives. The ocean color data set is a small, but important, constituent of NASA's Earth Science Program. The essence of that program can be summarized in five fundamental science questions (NASA, 2000). How is the global Earth system changing? What are the primary forcings of the Earth system? How does the Earth system respond to natural and human-induced changes? What are the consequences of change in the Earth system for human civilization? Finally, how well can we predict changes in the Earth system that will take place in the future? Ocean biogeochemistry plays a fundamental role in the Earth system, since through photosynthesis, the ocean's phytoplankton take up atmospheric carbon dioxide, sequestering it in the deep ocean, where it is slowly buried as sedimentary carbon. Currently, less than half of the carbon dioxide released into the atmosphere by combustion of fossil fuels and deforestation remains in the atmosphere. The remainder is sequestered in oceanic and terrestrial sinks. The ocean is part of a long-term biological buffering process for carbon, wherein various damping and feedback mechanisms in the Earth system regulate pulses of carbon from anthropogenic and natural sources. On a geologic time scale, the current anthropogenic release is a sudden pulse into the system. The buffering mechanisms are incompletely understood at best, and their capacity to cleanse the Earth system of the modern human pulse of carbon is not known.

For the oceans, an understanding of biogeochemical processes starts with a knowledge of the distribution and variability of phytoplankton in the surface waters of the world's oceans. The ocean color data set provides the basis for temporal and spatial variability studies with time periods from days to decades and with spatial sizes from mesoscale to global. The spatial scale requires the use of satellite-based observations, and the temporal scale requires the use of measurements from more than a single ocean color satellite instrument. These patterns of ocean phytoplankton concentrations provide a fundamental input to physical-biogeochemical process studies, including those of photosynthesis and respiration and of interactions at the air-sea interface. These processes are part of ocean primary production, the first step in the sequestering of excess atmospheric carbon dioxide. In addition, phytoplankton are the basic component of marine ecosystems, and phytoplankton patterns provide the basis for mesoscale and global marine ecosystem studies. We do not assume that the ocean color data set provides answers to the questions about the role of the oceans in the Earth system. However, the biological patterns in the data set provide information and understanding that are requisite to the development of those answers.

2.2. Operational Objectives. The calibration and validation programs for individual missions have a wide range of comprehensiveness, making international cooperation imperative to ensure high quality data. Fundamentally, the data set must have consistent products (chlorophyll-*a*, etc.) – consistent both in space and time. This implies a consistent derivation of those products, within the limitations of sensor-to-sensor differences. In other words, the pathway from the top-of-the-atmosphere radiance at the satellite instrument's input aperture to the geophysical data product should be as consistent as possible from instrument-to-instrument. Otherwise, it is problematic whether inconsistencies in the data products from different sources can be understood and rectified. And it is problematic whether an inconsistent ocean color data set will serve to meet the program's scientific objectives. There is, of course, no guarantee that a given pathway from top-of-the-atmosphere measurements to ocean data products is the optimal one. The evolution and improvement of the data set closely follows the development of improved algorithms. However, for any one version of the data set, a single consistent set of algorithms is essential.

There must be a temporal continuity – from satellite instrument to satellite instrument – in the data set. Sensor characterization and an effective, ongoing program of sensor calibration and validation are essential to separate the effects of changes in the ocean system from those from changes in the observing system. This is a particular challenge, since there are

few examples of continuous data records based on satellite measurements where data quality is consistent across changes in sensors, even when copies of the sensor design are used (NRC, 2000a). In the case of ocean color, only the two MODIS instruments have a common design. In addition, since the ocean color data set will be used to examine changes in ocean bio-optics over time periods of decades, it is imperative to preserve the calibration and operating information for each ocean color sensor, as well as metadata and ancillary data fields, in a manner that allows reprocessing. However, future reprocessings will require more than just the calibration data sets. For this reason, the SeaWiFS Project has developed an extensive set of technical memorandums to provide the information necessary to apply the calibration and validation techniques. Without such documentation, reprocessing attempts may prove problematical. These caveats for satellite measurements apply equally to the *in situ* instruments used to calibrate and validate them.

There must be a consistent, objective method for merging the data products from individual satellite instruments. In addition there must be a consistent, objective method for merging the data products from satellite and *in situ* instruments. The added value from *in situ* measurements makes their inclusion in the data set imperative. As with the data reduction algorithms, there is no guarantee that a given data merger scheme is the optimal one. And as with the case of algorithms, the evolution and improvement of the data set will follow the development of improved data merger methods. However, for any one version of the data set, a single consistent method of merging data products from different sources is essential.

Finally, as advocated by the US National Research Council for NASA's Post-2002 Earth observing missions, the ocean color data set should be developed under a sound scientific strategy – including supporting observational, data management, and analytical activities – that is: 1. Agile – to enable timely response to technological changes or to changing research priorities; 2. Focused – to enable progress on answering specific, central scientific questions about ocean bio-optical phenomena; and 3. Coherent – to enable a balanced (that is, space-based and *in situ*) and integrated, interagency and international response to ocean bio-optical issues (NRC, 1999b).

3. Implementation

Adaptability and flexibility are essential for the information system containing the ocean color data set if it is to be useful in a world of changing technical capabilities and scientific requirements. Current user demands on the system are generally known at best, and future user-driven needs are unknown. Similar considerations also apply to the data set, as well. It must be flexible enough to accommodate new data products that cannot yet be envisioned. And, in particular, it must have the capability for rapid reprocessing, starting from the on-orbit measurements and ending with the derived geophysical data set. For the creation of the ocean color data set, the SIMBIOS Program has developed a set of key tools: 1. a comprehensive bio-optical data base; 2. a program to evaluate different atmospheric correction algorithms; 3. a program to link the calibrations of individual ocean color satellite instruments; 4. a program (including calibration cross-calibrations and measurement protocols) to develop a consistent *in situ* calibration and validation data set for the satellite measurements; 5. alternate algorithms to convert radiometric measurements to derived geophysical products; and 6. alternate methods to combine ocean color measurements from different sources into a single data set.

3.1. Comprehensive Bio-Optical Data Base. Ground based measurements and measurement networks support and extend space-based observations. They are critical for algorithm development and for calibrating and validating satellite measurements. In addition, they often provide the high-resolution observations in both time and space needed to carry out the process studies that elucidate the mechanisms underlying ocean biochemistry. For example, Gregg and Conkright (2001) have combined about 70,000 surface observations with remotely-sensed data from the Coastal Zone Color Scanner (CZCS) to provide an enhanced set of seasonal chlorophyll-*a* climatologies for the CZCS era (1978-1986). The *in situ* and satellite data were merged using the Conditional Relaxation Analysis Method previously applied by Reynolds (1988) and Reynolds et al. (1989) to ameliorate biases in satellite sea surface temperature measurements. In one sense, the blended analysis of Gregg and Conkright (2001) uses the satellite chlorophyll-*a* field as an interpolation function for the *in situ* observations. In another sense, the blended analysis provides a vicarious calibration of the CZCS data products, which suffer from the limited success of the CZCS on-orbit radiometric calibration (Evans and Gordon, 1994). Generally, the CZCS appears to underestimate chlorophyll-*a* concentrations globally by 8 to 35%, and regionally, the blended analysis returns chlorophyll-*a* values that are often 20 to 40% and occasionally more than 100% greater than those from the CZCS (Gregg and Conkright, 2001). However, for large areas of the ocean gyres, the data merger was not possible, due to the lack of *in situ* observations. Ultimately, global ocean color data sets must be comprised of both *in situ* and space-based observations to ensure the optimal quality of the data.

In situ ocean measurements have an equally critical function in the development of the algorithms that convert radiometric measurements (water leaving radiance or surface reflectance) to geophysical data products (chlorophyll *a* and others). The quality of these conversion algorithms is no better than that of the data sets of ocean properties used to create them. The application of these algorithms to different oceanic locations (clear ocean basins or turbid coastal waters) is no better than the *in situ* data sets from the individual locations. And the development of these algorithms and of the associated

models of oceanic optical properties (Garver and Siegel, 1997, O'Reilley et al. 1998) is the reason for the radiometric measurements. In addition, subsequent *in situ* measurements will serve to validate ocean color algorithms after their development. *In situ* measurements are indispensable to any ocean color data set.

Since 1991, the SeaWiFS Project has worked to develop a database of *in situ* near-surface chlorophyll-*a* measurements – SeaBASS (the SeaWiFS Bio-optical Archive and Storage System) (Werdell et al. 2000). Since 1997, the original SeaWiFS database has been expanded to include *in situ* measurements by investigators and science team members of the SIMBIOS Program, making the archive a joint venture of the two projects. SeaBASS is a repository for *in situ* optical and pigment data products used for the validation of measurements from SeaWiFS and from other ocean color missions – and for the development of new ocean color algorithms. This latter function of SeaBASS is particularly important, since ocean color algorithm development is essentially limited by the availability of *in situ* measurements. Currently, the SeaBASS data set includes approximately 20,000 near surface chlorophyll-*a* measurements taken from more than 650 field campaigns. These data extend back to 1975, with the vast majority of the measurements from 1990 to date, and with new data received and placed in the archive on a regular basis.

All of the data from the field campaigns in SeaBASS is checked for proper formatting, relevant documentation, and associated calibration files. Some rudimentary quality control checks are run on the field data, and the results of these checks are resolved to the satisfaction of the experimenters.

SeaBASS includes a data archive and two relational databases (RDBs). The archive includes the near-surface chlorophyll-*a* measurements discussed above plus additional bio-optical data products, including phytoplankton pigments, total suspended particulate matter, and chromatic dissolved organic matter. As part of the SIMBIOS Project, the SeaBASS data archive has been expanded to include atmospheric measurements, principally aerosol optical thickness measurements from sun photometers. This archive can be searched using several online search engines and the bio-optical RDB. In addition, there is a separate historical pigment RDB, which contains over 300,000 records of phytoplankton pigment that can be searched online. The information in the historical pigment RDB is separate from the SeaBASS archive, and the historical pigment data are not currently maintained.

The historical pigment RDB is openly available to the public. However, access to the SeaBASS data archive and the bio-optical RDB are restricted to SeaWiFS Project and SIMBIOS Science Team members and to other approved individuals (including members of other ocean color instrument teams and voluntary data contributors) for advanced algorithm development and data product evaluation purposes. Further information on this policy and an application for a SeaBASS account registration are available at the SeaBASS website (<http://seabass.gsfc.nasa.gov>). The comparison of *in situ* chlorophyll-*a* measurements with SeaWiFS-derived values is discussed by Bailey et al. (2000) .

3.2. Atmospheric Correction Algorithm Evaluation. Current ocean color algorithms derive oceanic optical properties in a two step process, an atmospheric correction followed by a bio-optical algorithm to estimate the water properties. For ocean color measurements by satellite instruments, the greatest portion of the upwelling radiance at the top-of-the-atmosphere comes from the atmosphere itself. For the atmospheric correction algorithm, portions of the upwelling radiance, such as that part of the solar flux scattered upwards by air molecules, can be calculated exactly. However, the calculation of the upwelling radiance from atmospheric aerosols requires knowledge of both the aerosol type and amount. In current ocean color algorithms, the aerosol properties are determined using measurements in the near infrared, where the ocean surface is nearly black. Based on the properties determined from these measurements, a model of the aerosol type is selected from a set of candidate models, and the aerosol-based upwelling atmospheric radiance in the ocean color portion of the spectrum is calculated.

Current atmospheric correction algorithms, such as the one for SeaWiFS (Gordon and Wang, 1994), work reasonably well over most of the oceans, where the aerosols scatter the solar flux and absorb it weakly. However, there are regions, such as the Western Mid-Latitude North Pacific and the Eastern Tropical North Atlantic where the prevailing winds carry mineral-laden dust and anthropogenically-generated carbonaceous aerosols over the ocean. These aerosols absorb solar radiation in the ocean color portion of the spectrum, and the current atmospheric correction algorithms fail to account for it. This failure can be traced to two causes (Gordon, 1997). First, the spectral dependence of the aerosol scattering visible portion of the spectrum depends on the vertical distribution of the aerosol, whereas this is not the case in the near infrared where the aerosol properties are determined. Second, the spectral variation of aerosol scattering in the near infrared provides no information on the aerosol's absorbing characteristics, since they depends primarily on the aerosol's size distribution – a property that cannot be determined from the current set of near infrared measurements.

New, one-step ocean color algorithms are under development (Gordon et al. 1997, Chomko and Gordon, 1998). These algorithms retrieve the atmosphere and water properties simultaneously. These retrievals require both a first-guess aerosol model and a first-guess water model. There are fewer parameters in the models than there are measurement wavelengths by the ocean color instrument – and the model parameters are varied systematically until the difference between the measured and calculated results are minimized. The aerosol models use a three-component log-normal aerosol size distribution

(Shettle, 1984) or a Junge power-law distribution. Based on these distributions, the scattering and absorption properties are computed using Mie theory. These new one-step algorithms show a significant improvement in the atmospheric correction of ocean scenes containing absorbing aerosols. However, because of their iterative nature, these algorithms are currently too computer intensive for use with global ocean color data sets.

At the hearts of both the one-step and two-step ocean color algorithms are sets of aerosol models. The validation of the selection process for the aerosol models in these algorithms and the validation of the properties of the aerosols in the models are both central to the creation of an optimal ocean color data set. The principal source of *in situ* aerosol observations has been AERONET, the Aerosol Robotic Network (Holben et al. 1998), a network of ground-based automated sun photometers. Since the majority of the AERONET stations are at continental locations, the SIMBIOS Project has augmented the AERONET network with instruments at 13 additional coastal sites. The initial emphasis for SIMBIOS (Fargion et al. 2001) has been the use of the sun photometers for comparisons of *in situ* aerosol optical thicknesses with those derived from ocean color satellite measurements. Aerosol optical depth is a standard product of the atmospheric correction algorithms for the ocean color instruments, and it is a primary geophysical product for sun photometers. In addition, the SIMBIOS Project has concentrated on the development of protocols for the calibration of sun photometers and sky radiometers and of protocols for the analysis of the derived aerosol optical thicknesses, plus procedures for screening *in situ* optical thicknesses for comparisons with satellite-based measurements (Fargion et al. 2001). Comparisons of the *in situ* aerosol optical thicknesses with SeaWiFS results indicate a miscalibration of about 5% in the near infrared bands of the satellite instrument, giving satellite-based aerosol column amounts that are consistently greater than those from the sun photometers.

Sun and sky radiance measurements from the sun photometer instruments also provide optical properties for the atmospheric aerosols, properties that are basic to the atmospheric corrections of satellite ocean color measurements. In particular, a set of inversion algorithms has been developed that retrieves the aerosol size distribution over a wide range of sizes (0.05 to 15 μm) together with the spectrally dependent single-scattering albedo (Dubovik and King, 2000, Dubovik et al. 2000). The aerosol size distribution is a principal parameter in the atmospheric models for the one-step ocean color algorithms (Gordon et al. 1997, Chomko and Gordon, 1998), and the sun photometer derived distributions provide a valuable check of the assumptions within these algorithms. In addition, a climatology of aerosol size distributions at the SIMBIOS sites will provide a basis for refinements to the atmospheric correction portions of the one-step algorithms. Results for the aerosol size distribution and single scattering albedo at the SIMBIOS site in Bahrain (Smirnov et al. 2001) provide a start for these climatologies.

For the current, two-step ocean color algorithms, the single scattering albedo is the principal aerosol property derived from the satellite instrument's measurements in the near infrared (Gordon and Wang, 1994), and it is the wavelength dependence of the algorithm-based albedo that is used to provide the aerosol-based upwelling atmospheric radiance for the ocean color bands. As with the aerosol size distributions, the *in situ* single scattering albedos provide an independent check of the ocean color algorithms, as well as the climatological basis for improved scattering models in the algorithms. The atmospheric portion of the SeaWiFS two-step ocean color algorithm continues to be improved and updated (Wang, 2000). The SIMBIOS Project is pursuing the use of sun photometer results in this process. It is anticipated that these studies can be applied to the atmospheric algorithms for other ocean color instruments as well.

3.3. Satellite Instrument Calibration. For long-term measurements of climate variables, effective on-going programs of sensor calibration and validation, sensor characterization, data continuity, and strategies for ensuring overlap across successive sensors are essential (NRC, 2000a). Individual ocean color satellite instruments use individual characterization and calibration methods, and there will be differences in the on-orbit measurements from these instruments. A multi-platform ocean color data set requires a means of unifying measurements from different satellite sensors. For example, as part of the pre-flight calibration activities for OCTS and SeaWiFS, the SeaWiFS Transfer Radiometer (SXR) was used as part of a radiometric measurement comparison of the integrating sphere used to calibrate OCTS (Johnson et al. 1997) and as a calibration standard for the SeaWiFS integrating sphere (Johnson et al. 1999). The EOS Project has developed a similar transfer radiometer to cross-calibrate MODIS, the other EOS sensors, GLI, and MERIS. These round-robin measurements serve to link the prelaunch radiometric calibrations of different ocean color satellite instruments. It is also important to understand the operating characteristics of the satellite instruments, such as their susceptibility to spatial stray light from bright targets (clouds and land surfaces) adjacent to ocean scenes. For the SeaWiFS sensor, the instrument characterization has been extensively documented in the SeaWiFS technical memorandum series. In addition, the SIMBIOS Project is proceeding to unify the on-orbit calibration of SeaWiFS with other instruments using water-leaving radiances from MOBY as a surface truth reference. This process does not preclude the need for surface truth measurements at other sites, nor does it preclude the need for a thorough characterization of each satellite sensor, nor does it preclude the need for an active program of on-orbit calibration for each sensor.

3.3.1. Direct On-Orbit Calibration. Individual ocean color instruments use a variety of techniques for determining the calibration of their measurements on orbit and monitoring changes in sensor performance. For OCTS, the on-orbit calibration relied primarily on internal calibration lamps and on underflights by a calibrated airborne sensor as an absolute reference (Shimada et al. 1999). For POLDER, the in-flight radiometric calibration did not rely on any on-board calibration device (Hagolle et al. 1999). POLDER used atmospheric molecular scattering as an absolute reference and used measurements of ocean sun glint and high altitude cloud-tops for relative (band-to-band) calibrations. In addition, POLDER used measurements of a set of ground sites to monitor changes in the instrument over time. For SeaWiFS, the laboratory calibration was carried to orbit using the transfer-to-orbit experiment (Barnes et al. 2000), and instrument changes are determined by using the moon as an external diffuse reflector (Barnes et al. 1999). For SeaWiFS, the only absolute portion of the calibration chain is the calibration in the laboratory before launch. For MODIS, and for several instruments to follow, the on-orbit calibration reference is an onboard diffuse reflecting plaque, the changes of which are determined by a ratioing radiometer (Guenther et al. 1996). For each of these instruments, the estimated uncertainty in the top-of-the-atmosphere measurements is about 5% or less, and for each of these instruments there is a record of its characterization and calibration.

3.3.2. Vicarious Calibration. With the review of the Coastal Zone Color Scanner (CZCS) calibration by Evans and Gordon (1994), it has become clear that onboard measurements alone are inadequate to provide good ocean color measurements. In principle, this is due to the nature of the measurements. In the visible, the ocean is dark, and the majority of the flux at the top-of-the-atmosphere (90% or more) comes from the atmosphere. Since the removal of the atmospheric radiance is an essential part of ocean color measurements, the radiance from the ocean is calculated as the small difference between two large values. Thus, an error of 1% in the top-of-the-atmosphere radiance can cause an error of 10% or more in the derived radiance at the ocean surface. As a result, the SeaWiFS ocean color data are vicariously calibrated. Here, the term vicarious has the definition – “as seen through the eyes of another.” SeaWiFS data are calibrated at a single point on the globe, off the Hawaiian Island of Lanai, using comparisons with the water-leaving radiances from the MOBY buoy (Clark et al. 1997). For the visible bands, vicarious calibration coefficients adjust the top-of-the-atmosphere radiances from the instrument until the derived water-leaving radiances agree with those from MOBY. This is a calibration of the “instrument/atmospheric correction algorithm system” for SeaWiFS, since both parts of the system are required to derive the water-leaving radiance. Included in the SeaWiFS Post-Launch technical memorandum series (McClain et al. 2000a, 2000b) are outlines of the suite of procedures and quality control tests used for the postlaunch calibration and validation of SeaWiFS.

The SIMBIOS Project has developed software for processing measurements from several ocean color sensors. This set of algorithms (MSL12) is based on the standard SeaWiFS atmospheric correction (Gordon and Wang, 1994, Wang, 2000). It can be applied to other sensors, such as OCTS and POLDER, giving a consistent atmospheric correction for each instrument. Since OCTS and POLDER flew in tandem on the ADEOS spacecraft and made several measurements of the MOBY site during their operational lifetimes, Wang et al. (2001) have performed a vicarious calibration of these instruments using *in situ* data from MOBY. After the calibration, there are no obvious differences in the OCTS and POLDER-derived ocean products, based on common measurements by the two instruments over the Sargasso Sea and the Bermuda area. These results indicate that the OCTS and POLDER ocean color sets data can be compared and merged in the sense that there is no significant bias between them. These results also indicate that it may be possible to cross-calibrate instruments on different spacecraft – such as SeaWiFS and MODIS – using MOBY as a common calibration reference. In this case, a detailed analysis by the SIMBIOS Project is probably unnecessary, since MODIS ocean color data products are vicariously calibrated at MOBY, in a manner similar to SeaWiFS.

3.4. *In situ* Instrument Calibration and Protocols. Ground based measurements are critical for calibrating and validating ocean color measurements from space. The SIMBIOS Project is continuing the series of SeaWiFS intercalibration round-robin experiments (Johnson et al. 1999) with a program cross-calibrations of laboratory sources using a travelling transfer radiometer, the SXR2. This instrument is a second-generation version of the SXR, which was used in a radiometric measurement comparison of the OCTS visible and near infrared integrating sphere (Johnson et al. 1997) as part of the pre-flight calibration and validation activities for OCTS and SeaWiFS. The SXR2 shares the spectral responses of the SXR; however, the SXR2 has been designed to view reference sources for *in situ* ocean color instruments, reference sources that are less bright than those used to calibrate satellite instruments. The SXR2 was calibrated in early 2001 at the NIST facility for Spectral Irradiance and Radiance Responsivity Calibrations with Uniform Sources (SIRCUS) (Brown et al. 2000). SIRCUS used tuneable laser sources to provide monochromatic light flux for the set of wavelengths over the spectral response ranges of the SXR2. In addition, the SXR2 was calibrated at NIST using a standard broadband source. This year, SXR2 cross calibration measurements have been made at the US Naval Research Laboratory, the Scripps Institute of Oceanography, and the University of California Santa Barbara. Comparisons with other institutions are being scheduled. The SIMBIOS Project has developed the SXR2 as a cross-calibration tool for use by the ocean color community.

The continuity and consistency of the global data set is a direct reflection of the continuity and consistency of the *in situ* measurements used to calibrate and validate it. This is the premise for the SIMBIOS cross-calibration program. In addition, a standard set of measurement protocols is indispensable for the required consistency in the *in situ* calibration data set. The development of *in situ* measurement protocols has been a primary focus of both the SeaWiFS and SIMBIOS Projects (see Fargion and Mueller (2000) and the references cited therein). It continues as a primary focus in the development of the multi-sensor global ocean color data set.

4. Creating a Multi-Sensor Global Ocean Color Data Set

The work of Wang et al. (2001) has demonstrated the feasibility of merging the ocean color data sets from OCTS and POLDER. And the SIMBIOS Program is using the measurements from these instruments to test techniques for merging global data sets. However, the operational lifetimes of these instruments (November 1996 to June 1997) do not overlap with those from the current series of global ocean color instruments. Currently, the investigations of merger techniques for derived ocean color data products, particularly chlorophyll-*a*, center on four approaches (Gregg, 2001): a simple splicing and averaging of measurements from two or more satellite instruments; a subjective analysis, where specific deficiencies of individual sensors are identified and used to weight the results from the mergers; the application of the Conditional Relaxation and Analysis method used by Gregg and Conkright (2001) to merge CZCS satellite measurements with *in situ* results; and an optimal interpolation method designed to maintain continuity within the merged data set. Each approach has strengths and weaknesses, and each has been applied, in a preliminary manner, to measurement results from SeaWiFS and MODIS. Refinements of these analyses will continue as reprocessed, science-quality MODIS ocean color measurements become available in the second half of 2001.

In addition, the SIMBIOS Program is investigating the use of semi-analytical in-water algorithms as a basis for merging measurements from multiple satellite instruments (Siegel and Maritorena, 2000). In this approach, the algorithm is adapted to convert the radiometric results from each ocean color instrument's measurements (water-leaving radiance or remote sensing reflectance) into the optical properties of the water (the coefficients for absorption and backscattering). And from these properties, the derived ocean color products, including chlorophyll-*a*, are derived. The use of a semi-analytical model allows the merger of the measurements at the level of the radiometric measurements, rather than at the level of the derived geophysical products. This approach gives a single, consistent method for deriving geophysical products from the radiometric measurements of the instruments. It can be adapted to individual satellite and *in situ* sensors, since it can be adapted for the different measurement wavelengths of different instruments. However, this approach also requires a single, consistent atmospheric correction algorithm and a single in-water bio-optical model.

Presently, we are unable to evaluate fully the relative advantages of these two basic merger techniques – merger at the level of the derived data products (the outputs of individual in-water algorithms from individual instruments) or merger at the level of the radiometric measurements (the inputs of individual instruments to a common in-water algorithm). The development of these merger techniques remains an active research area for the SIMBIOS Program.

5. Concluding Remarks

The SIMBIOS Program has solicited advice from the IOCCG on the merger of multi-platform ocean color measurements, including the spatial and temporal resolution of the derived data set. The IOCCG has been actively involved with the issues surrounding complementary ocean color missions (IOCCG, 1999). It is anticipated that a partnership between the IOCCG and the SIMBIOS Program will lead to a data set that meets the needs of the international ocean color community. However, the coordination of a long-term multi-platform ocean color data set by the SIMBIOS Program and the IOCCG is a scientific and technological experiment requiring collaboration by the international community. The SIMBIOS Program has developed a set of tools and procedures to initiate such a data set. However, we recognize that, along with its usefulness, there will be deficiencies in it. We anticipate that the improvements to this ocean color data set will come from collaborations with our colleagues within – and without of – the SIMBIOS Program. It is a work in progress.

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